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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
09/773,281	01/31/2001	Steven L. Dixon	PHARMA.002A2	1986
20995	7590	08/31/2005	EXAMINER	
KNOBBE MARTENS OLSON & BEAR LLP 2040 MAIN STREET FOURTEENTH FLOOR IRVINE, CA 92614			HIRL, JOSEPH P	
			ART UNIT	PAPER NUMBER
			2129	

DATE MAILED: 08/31/2005

Please find below and/or attached an Office communication concerning this application or proceeding.

**Office Action Summary**

Application No.

09/773,281

Applicant(s)

DIXON ET AL.

Examiner

Joseph P. Hirl

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-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

**Period for Reply**

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If the period for reply specified above is less than thirty (30) days, a reply within the statutory minimum of thirty (30) days will be considered timely.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

**Status**

- 1) ☒ Responsive to communication(s) filed on 20 June 2005.
- 2a) ☒ This action is **FINAL**. 2b) ☐ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

**Disposition of Claims**

- 4) ☒ Claim(s) 1-35 is/are pending in the application.
- 4a) Of the above claim(s) \_\_\_\_\_ is/are withdrawn from consideration.
- 5) ☐ Claim(s) \_\_\_\_\_ is/are allowed.
- 6) ☒ Claim(s) 1-35 is/are rejected.
- 7) ☐ Claim(s) \_\_\_\_\_ is/are objected to.
- 8) ☐ Claim(s) \_\_\_\_\_ are subject to restriction and/or election requirement.

**Application Papers**

- 9) ☐ The specification is objected to by the Examiner.
- 10) ☒ The drawing(s) filed on 29 March 2002 is/are: a) ☒ accepted or b) ☐ objected to by the Examiner.  
Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).  
Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
- 11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

**Priority under 35 U.S.C. § 119**

- 12) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☐ All b) ☐ Some \* c) ☐ None of:
1. ☐ Certified copies of the priority documents have been received.
  2. ☐ Certified copies of the priority documents have been received in Application No. \_\_\_\_\_.
  3. ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).
- \* See the attached detailed Office action for a list of the certified copies not received.

**Attachment(s)**

- |  |   |
|--|---|
| 1) <input type="checkbox"/> Notice of References Cited (PTO-892)   | 4) <input type="checkbox"/> Interview Summary (PTO-413)<br>Paper No(s)/Mail Date. _____ |
| 2) <input type="checkbox"/> Notice of Draftsperson's Patent Drawing Review (PTO-948)                                   | 5) <input type="checkbox"/> Notice of Informal Patent Application (PTO-152)             |
| 3) <input type="checkbox"/> Information Disclosure Statement(s) (PTO-1449 or PTO/SB/08)<br>Paper No(s)/Mail Date _____ | 6) <input type="checkbox"/> Other: _____  |

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### **DETAILED ACTION**

1. This Office Action is in response to an AMENDMENT entered June 20, 2005 for the patent application 09/773,281 filed on January 31, 2001.
2. The First Office Action of March 17, 2005 is fully incorporated into this Final Office Action by reference.

### ***Status of Claims***

3. Claims 1-35 are pending.

### ***Double Patenting***

4. A rejection based on double patenting of the "same invention" type finds its support in the language of 35 U.S.C. 101 which states that "whoever invents or discovers any new and useful process ... may obtain a patent therefor..." (Emphasis added). Thus, the term "same invention," in this context, means an invention drawn to identical subject matter. See *Miller v. Eagle Mfg. Co.*, 151 U.S. 186 (1894); *In re Ockert*, 245 F.2d 467, 114 USPQ 330 (CCPA 1957); and *In re Vogel*, 422 F.2d 438, 164 USPQ 619 (CCPA 1970).

A statutory type (35 U.S.C. 101) double patenting rejection can be overcome by canceling or amending the conflicting claims so they are no longer coextensive in

scope. The filing of a terminal disclaimer cannot overcome a double patenting rejection based upon 35 U.S.C. 101.

5. Claims 12-21 and 23-34 are provisionally rejected under 35 U.S.C. 101 as claiming the same invention as that of claims 1-35 of copending Application No. 09/770,510. This is a provisional double patenting rejection since the conflicting claims have not in fact been patented.

6. The nonstatutory double patenting rejection is based on a judicially created doctrine grounded in public policy (a policy reflected in the statute) so as to prevent the unjustified or improper timewise extension of the "right to exclude" granted by a patent and to prevent possible harassment by multiple assignees. See *In re Goodman*, 11 F.3d 1046, 29 USPQ2d 2010 (Fed. Cir. 1993); *In re Longi*, 759 F.2d 887, 225 USPQ 645 (Fed. Cir. 1985); *In re Van Ornum*, 686 F.2d 937, 214 USPQ 761 (CCPA 1982); *In re Vogel*, 422 F.2d 438, 164 USPQ 619 (CCPA 1970); and, *In re Thorington*, 418 F.2d 528, 163 USPQ 644 (CCPA 1969).

A timely filed terminal disclaimer in compliance with 37 CFR 1.321© may be used to overcome an actual or provisional rejection based on a nonstatutory double patenting ground provided the conflicting application or patent is shown to be commonly owned with this application. See 37 CFR 1.130(b).

Effective January 1, 1994, a registered attorney or agent of record may sign a terminal disclaimer. A terminal disclaimer signed by the assignee must fully comply with 37 CFR 3.73(b).

7. Claims 1-11, 22 and 35 are provisionally rejected under the judicially created doctrine of double patenting over claims 1-11, 20-22 and 35 of copending Application No. 09/770,510. This is a provisional double patenting rejection since the conflicting claims have not yet been patented.

The subject matter claimed in the instant application is fully disclosed in the referenced copending application and would be covered by any patent granted on that copending application since the referenced copending application and the instant application are claiming common subject matter, as follows: Claims 1-11, 22: selected atoms have assigned positions without positions being assigned; Claim 35: the molecule of concern is the related molecule.

Furthermore, there is no apparent reason why applicant would be prevented from presenting claims corresponding to those of the instant application in the other copending application. See *In re Schneller*, 397 F.2d 350, 158 USPQ 210 (CCPA 1968). See also MPEP § 804.

### ***Claim Rejections – 35 USC § 102***

8. The following is a quotation of the appropriate paragraphs of 35 U.S.C. 102 that form the basis for the rejections under this section made in this Office action:

A person shall be entitled to a patent unless –

(e) the invention was described in (1) an application for patent, published under section 122(b), by another filed in the United States before the invention by the applicant for patent or (2) a patent granted on an application for patent by another filed in the United States before the invention by the applicant for patent, except that an international application filed under the treaty defined in section 351(a) shall have the effects for purposes of this subsection of an application filed in the United States

only if the international application designated the United States and was published under Article 21(2) of such treaty in the English language.

9. Claims 1-35 are rejected under 35 U.S.C. 102(e) as being anticipated by Agrafiotis, et al (U. S. Patent 6,453,246, referred to as **Agrafiotis**).

**Claims 1, 35**

Agrafiotis anticipates deriving a first one-dimensional representation of a first molecule from distances between selected atoms of said first molecule, wherein the selected atoms of the first molecule are assigned positions in the first one-dimensional representation (**Agrafiotis**, c 6, l 1-6; c 6, 18-20; Examiner's Note (EN); the "wherein" statement does not provide further limitation since it was necessary to know the positions of the atoms to determine the distance); deriving a second one-dimensional representation of a second molecule from distances between selected atoms of said second molecule wherein the selected atoms of the second molecule are assigned positions in the second one-dimensional representation (**Agrafiotis**, c 6, l 1-6; c 6, 18-20; EN: the "wherein" statement does not provide further limitation since it was necessary to know the positions of the atoms to determine the distance); and comparing said one dimensional representations (**Agrafiotis**, c 6, l 39-47; EN: first and second molecule will have chemical properties; a set of atoms can each have a unique spatial identity and the relationship between them is a straight line ... a linear representation ).

**Claims 2, 34**

Agrafiotis anticipates said one-dimensional representations comprise linear representations (**Agrafiotis**, c 15, l 37-44).

**Claim 3**

Agrafiotis anticipates said deriving comprises calculating a linear position for each of a plurality of selected atoms of said first molecule (**Agrafiotis**, c 15, l 56-65).

**Claim 4**

Agrafiotis anticipates wherein said linear positions are selected to reduce the deviation between relative positions of said plurality of selected atoms along a line and three dimensional distances between said plurality of atoms in said first molecule(**Agrafiotis**, c 15, l 56-65).

**Claim 5**

Agrafiotis anticipates calculating a linear position for each of a plurality of selected atoms of said second molecule (**Agrafiotis**, c 15, l 56-65).

**Claim 6**

Agrafiotis anticipates said comparing comprises aligning said one dimensional representations so as to match linear positions of at least one of said selected atoms of said first molecule with at least one of said selected atoms of said second molecule (**Agrafiotis**, c 15, l 56-65).

**Claim 7**

Agrafiotis anticipates said matched atoms have the same element type (**Agrafiotis**, c 12, l 58-67).

**Claim 8**

Agrafiotis anticipates said matched atoms have the same hybridization state (**Agrafiotis**, c 12, l 58-67).

**Claim 9**

Agrafiotis anticipates at least some of said distances are derived from molecular topology (**Agrafiotis**, c 14, l 1-10).

**Claim 10**

Agrafiotis anticipates at least some of said distances are derived from bond counts (**Agrafiotis**, c 12, l 58-67).

**Claim 11**

Agrafiotis anticipates at least some of said distances are derived from three dimensional atomic coordinates (**Agrafiotis**, c 15, l 37-44).

**Claim 12**

Agrafiotis anticipates representing a first molecule as a first set of selected atoms, wherein each atom of said first set is associated with an atom type and a scalar value, wherein the scalar values are derived from distances between said selected atoms (**Agrafiotis**, c 6, l 1-6; c 6, 18-20); representing a second molecule as a second set of selected atoms, wherein each atom of said second set is associated with an atom type and a scalar value, wherein the scalar values are derived from distances between said selected atoms (**Agrafiotis**, c 6, l 1-6; c 6, 18-20); and comparing said atom types and scalar values (**Agrafiotis**, c 6, l 39-47).

**Claims 13, 24**

Agrafiotis anticipates said scalar value represents a linear position (**Agrafiotis**, c 15, l 37-44).



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**Claims 14, 25**

Agrafiotis anticipates each atom of said set is associated with a second scalar value, said second scalar value representing a width centered about each of said linear positions (**Agrafiotis**, c 15, l 37-44; EN: seep p 11. below; width is the radius - distance to a related atom)..

**Claim 15**

Agrafiotis anticipates wherein said comparing comprises: aligning the linear positions of an atom in the first molecule with an atom of the same type in the second molecule such that their lengths completely overlap (**Agrafiotis**, c 19, l 5-16); and evaluating the amount of overlap between atoms of the first molecule and atoms of the same type of the second molecule (**Agrafiotis**, c 19, l 5-16; EN: such is dissimilarity).

**Claim 16**

Agrafiotis anticipates repeating the aligning and evaluating steps so as to evaluate the overlap at all linearly aligned positions of atom pairs having the same type (**Agrafiotis**, c 19, l 5-16).

**Claims 17, 26**

Agrafiotis anticipates said second scalar value is the same for all of said selected atoms (**Agrafiotis**, c 19, l 5-16; EN: such will be the case when the atoms are the same).

**Claims 18, 20**

Agrafiotis anticipates representing a non-linear three dimensional configuration of a molecule made up of a plurality of bonded atoms, said method comprising assigning,

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to at least some of said atoms, a position along a line so as to define a set of linear distances between each of said selected atoms, wherein at least some of said linear distances are not equal to the corresponding three dimensional distances between the same atoms in said molecule (**Agrafiotis**, c 12, l 58-67; c 13, l 1-7; c 15, l 37-44; EN: topologic features are defined by three dimensions).

### **Claims 19, 21, 31**

Agrafiotis anticipates reducing a total deviation between said set of linear distances and the corresponding three dimensional distances between the same atoms in said molecule (**Agrafiotis**, c 15, l 24-65).

### **Claim 22**

Agrafiotis anticipates storing linear representations of said molecular structures in a database, said linear representations being derived from three dimensional distances or topological distances between atoms of said molecular structures, wherein at least some of the atoms of each molecular structure are assigned positions in the respective linear representations (**Agrafiotis**, c 15, l 56-65; Fig. 1; c 6, l 1-2; EN: the “wherein” statement does not provide further limitation since it was necessary to know the positions of the atoms to determine the linear representations); deriving a linear representation of a molecule having known biochemical activity from three dimensional distances, or topological distances between atoms of said molecule, wherein at least some of the atoms of each molecular structure are assigned positions in the respective linear representations (**Agrafiotis**, c 15, l 56-65; Fig. 1; c 6, l 1-15; EN: the “wherein” statement does not provide further limitation since it was necessary to know the

positions of the atoms to determine the linear representations); comparing said linear representation of said molecule having known biochemical activity with said linear representations of said molecular structures in said database (**Agrafiotis**, c 5, l 56-65; c 6, l 28-47).

**Claim 23**

Agrafiotis anticipates selecting a set of atoms in said molecule (**Agrafiotis**, c 6, l 1-15); deriving a set of scalar values from distances between said selected atoms (**Agrafiotis**, c 6, l 1-6; c 6, l 18-20); assigning to each of said selected atoms a parameter set including an atom type and one of said set of scalar values (**Agrafiotis**, c 15, l 56-65; EN: coordinates are parameters).

**Claims 27, 28, 32, 33**

Agrafiotis anticipates said distances comprise three dimensional distances (**Agrafiotis**, c 13, l 1-3; EN: topologic features are defined in three dimensions).

**Claim 29**

Agrafiotis anticipates comparing molecules that have been parameterized according to the method of Claim 23 (**Agrafiotis**, c 15, l 56-65).

**Claim 30**

Agrafiotis anticipates a computer readable storage medium having stored thereon structural representations of molecules for retrieval by a computer implemented molecular screening program, wherein at least one of said structural representations comprises a list of selected atoms in said molecule, wherein each of said selected

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atoms is associated with an atom type and a scalar value (Agrafiotis, Fig. 1 & 2;

abstract; c 6, l 1-6).

### ***Response to Arguments***

10. The rejection of claims 1-11 and 18-29 under 35 USC 101 are withdrawn.

11. Applicant's arguments filed on June 20, 2005 related to Claims 1-35 have been fully considered but are not persuasive.

In reference to Applicant's argument:

The Examiner provisionally rejected Claims 1-35 under 35 U.S.C. § 101 for statutory double patenting relative to co-pending Application No. 091770,510. The Applicants believe it is appropriate to wait until either the claims in the instant application or the co-pending application are otherwise in condition for allowance to address the double-patenting rejections. See M.P.E.P. § 804(1)(B) ("The 'provisional' double patenting rejection should continue to be made by the examiner in each application...unless that 'provisional' double patenting rejection is the only rejection remaining in one of the applications. If the 'provisional' double patenting rejection in one application is the only rejection remaining in that application, the examiner should then withdraw that rejection and permit the application to issue").

Examiner's response:

In accordance with the MPEP, the appropriate double patenting rejections remain.

In reference to Applicant's argument:

The Examiner rejected Claims 1-35 under 35 U.S.C. § 102(e) as being anticipated by U.S. Patent No. 6,453,246 (Agrafiotis et al.). Agrafiotis discloses representing objects (e.g., molecules) as points in a multi-dimensional space. E.g., abstract ("points in a multi-dimensional space"); col. 5, lines 49-50 ("objects ...represent[ed] in a multi-dimensional space"); col. 11, lines 65-66 ("objects ...represented as vectors in multi-variate property space"); col. 19, lines 9-10 ("The display map has a point for each of the selected compounds."). As such, each object representation in Agrafiotis will consist of a single point characterized by a plurality of coordinates. Comparisons between multiple objects are evaluated by the distance in the multi

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dimensional space between the points associated with each object. See e.g., col. 5, lines 29-33. In contrast, molecules in the present invention are represented by positioning atoms of the molecules in one-dimensional representations. Agrafiotis does not disclose representing individual atoms in a one-dimensional representation of a molecule.

Specifically, Claim 1 requires one-dimensional representations of molecules where selected atoms of the molecules are assigned positions in the representations. Agrafiotis does not disclose representations of a molecule where individual atoms are positioned in the representation. Instead, whole molecules are represented by single points in a multi-dimensional property space without reference to individual atoms in the molecule.

Examiner's response:

Para 15. applies. The scalar or single dimension representation of claim 1 is derived from pair-wise relationships and such concept is taught by Agrafiotis @ c 6, lines 39-47 (EN: a pair of atoms are selected for a given molecule).

In reference to Applicant's argument:

Claims 12, 23, and 30 require associating or assigning a scalar value (e.g., a one dimensional coordinate) to individual atoms in a molecule. Agrafiotis also does not disclose assigning coordinates to individual atoms within a molecule but rather assigns coordinates to the molecule as a whole. E.g., col. 19, lines 9-10 ("The display map has a point for each of the selected compounds."). Accordingly, Claims 12, 23, and 30 and dependent Claims 13-17, 24-29, and 31-34 are not anticipated by Agrafiotis.

Claims 18 and 20 require assigning to atoms in a molecule a position (e.g., a coordinate) along a line (e.g., a one-dimensional representation). As discussed above, Agrafiotis does not disclose assigning positions to individual atoms within a molecule.

Examiner's response:

Pair-wise evaluation meets the limiting criteria of claims 12, 23 and 30 and is anticipated by Agrafiotis @ c 6, lines 39-47. Each item of a pair-wise set can have the same scalar value or distance between the related set. A line is a two-dimensional representation. A atom is an object and Agrafiotis determines distance on a display map which equates to having atoms or objects on a line (Agrafiotis, c 9, l 2-4).

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In reference to Applicant's argument:

Claim 22 requires deriving linear representations of molecules where at least some of the atoms in the molecules are assigned positions in the linear representation. As already noted, Agrafiotis does not disclose assigning individual atoms in a molecule to positions in a linear representation. Instead, whole molecules are represented by a single point in a multi-dimensional property space without reference to individual atoms in the molecule.

Examiner's response:

See the discussion above.

In reference to Applicant's argument:

Claims 35 requires retrieving linear representations of molecules where the representations comprise a set of atoms and associated linear positions in the linear representation. Agrafiotis does not disclose representing linear positions of individual atoms in a molecule in a linear representation. Instead, whole molecules are represented by a single point in a multi-dimensional space. Accordingly, Claim 35 is not anticipated by Agrafiotis.

Examiner's response:

Para 15. applies. Pair-wise evaluation meets the limiting criteria and is anticipated by Agrafiotis @ c 6, lines 39-47. Each item of a pair-wise set, object or atom, can have the same scalar value or distance between the related set. The line connecting such objects is a linear representation. An atom is an object and Agrafiotis determines distance on a display map which equates to having atoms or objects on a line (Agrafiotis, c 9, l 2-4).

### ***Examination Considerations***

12. The claims and only the claims form the metes and bounds of the invention.

"Office personnel are to give the claims their broadest reasonable interpretation in light

of the supporting disclosure. *In re Morris*, 127 F.3d 1048, 1054-55, 44USPQ2d 1023, 1027-28 (Fed. Cir. 1997). Limitations appearing in the specification but not recited in the claim are not read into the claim. *In re Prater*, 415 F.2d, 1393, 1404-05, 162 USPQ 541, 550-551 (CCPA 1969)" (MPEP p 2100-8, c 2, I 45-48; p 2100-9, c 1, I 1-4). The Examiner has full latitude to interpret each claim in the broadest reasonable sense. Examiner will reference prior art using terminology familiar to one of ordinary skill in the art. Such an approach is broad in concept and can be either explicit or implicit in meaning.

13. Examiner's Notes are provided to assist the applicant to better understand the nature of the prior art, application of such prior art and, as appropriate, to further indicate other prior art that maybe applied in other office actions. Such comments are entirely consistent with the intent and spirit of compact prosecution. However, and unless otherwise stated, the Examiner's Notes are not prior art but a link to prior art that one of ordinary skill in the art would find inherently appropriate.

14. Unless otherwise annotated, Examiner's statements are to be interpreted in reference to that of one of ordinary skill in the art. Statements made in reference to the condition of the disclosure constitute, on the face of it, the basis and such would be obvious to one of ordinary skill in the art, establishing thereby an inherent prima facie statement.

15. Examiner's Opinion: paras 12-14 apply. The Examiner has full latitude to interpret each claim in the broadest reasonable sense.

***Conclusion***

16. Applicant's amendment necessitated the new ground(s) of rejection presented in this Office action. Accordingly, **THIS ACTION IS MADE FINAL**. See MPEP § 706.07(a). Applicant is reminded of the extension of time policy as set forth in 37 CFR 1.136(a).

A shortened statutory period for reply to this final action is set to expire **THREE MONTHS** from the mailing date of this action. In the event a first reply is filed within **TWO MONTHS** of the mailing date of this final action and the advisory action is not mailed until after the end of the **THREE-MONTH** shortened statutory period, then the shortened statutory period will expire on the date the advisory action is mailed, and any extension fee pursuant to 37 CFR 1.136(a) will be calculated from the mailing date of the advisory action. In no event, however, will the statutory period for reply expire later than **SIX MONTHS** from the date of this final action.

17. Claims 1-35 are rejected.

***Correspondence Information***

Any inquiry concerning this information or related to the subject disclosure should be directed to the Examiner, Joseph P. Hirl, whose telephone number is (571) 272-3685. The Examiner can be reached on Monday – Thursday from 6:00 a.m. to 4:30 p.m.



If attempts to reach the Examiner by telephone are unsuccessful, the Examiner's supervisor, Anthony Knight can be reached at (571) 272-3687.

Any response to this office action should be mailed to:

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Joseph P. Hirl  
Primary Examiner, August 23, 2005